National Institute of Standards and Technology
U.S. Department of Commerce

MEASUREMENT SCIENCE FOR

Sustainable Infrastructure Materials

What is the problem?

National and international economic growth cannot continue into the next century unless industries, especially high volume trades like the construction industry, dramatically reduce the amounts of natural resources and energy they consume and the waste that they produce. To remain globally competitive while embracing sustainability, the U.S. construction industry needs to reexamine and redefine its practices: chemicals, materials, manufacturing methods, products, and waste disposal. Currently, construction materials, mainly concrete, steel, and polymeric materials, are being consumed at an annual rate of approximately $500 billion per year in new construction, and an additional $2.2 trillion in materials and construction products are required for renewal of the existing deteriorating U.S. physical infrastructure, according to the 2009 American Society of Civil Engineers Infrastructure Report Card.

Sustainability drivers include energy costs, global climate change, environmental regulations, disposal costs, resource scarcities, and population increases. Examples of environmental concerns include the need to reduce environmental impact through the inclusion of increased fractions of supplementary cementitious materials, like fly ash (one of the residues generated in the combustion of coal) and slag (a byproduct of metal smelting), into concrete as well as reduce environmental, health, and safety concerns related to the potential release of nanoparticles from nanocomposite materials that are rapidly being introduced into the marketplace.

Sustainability decision analysis tools are currently being developed by industry, government agencies, and standards organizations. The efficacy of these decision tools, however, is greatly hampered by the lack of reliable sustainability input data, especially service life data for materials, components and systems, and the absence of measurement science for gauging this critical input. Without technically sound, thoroughly evaluated measurement science, the input available for making sustainability decisions is too crude and unreliable. This deficiency was highlighted at a recent meeting hosted by the U.S. Department of Commerce where industry expressed the "need for the establishment of internationally comparable metrics to measure the cost-effectiveness of sustainable manufacturing practices."

Why is it hard to solve?

The most fundamental quality in full-life cycle assessment is a reliable estimate of the expected service life of a material, component, or system. Current durability tests were designed early in the 20th century to make qualitative performance assessments (i.e., at best, they can provide assessments as to whether product A is better than product B or vice versa under a specified set of exposure conditions) and these tests are fraught with scientific uncertainties. Extensive research efforts are being made to put service life estimation on a scientific basis. The measurement science needed to generate quantitative and accurate predictions of service life, however, is at a nascent level.

The measurement science for predicting the service life of construction materials involves measurements of the degradation, flammability, and nanoparticle release from these materials. These processes are inherently complex. They involve numerous component interactions and multifunctional (chemical, physical, and mechanical) responses that operate over extremely wide length and time scale ranges. Nanoscale materials also possess unique properties (high surface area, high surface reactivity, large inter-particle forces) that will affect degradation, flammability, and the release rate of nanoparticles in unknown ways. Science-based models for predicting these complex phenomena are just beginning to be developed, but such modeling is known to involve multiscale, multifunctional interactions in which damage accumulates over time. A multiplicity of linked models will be necessary to span these length and time scales, which in turn require advanced, high resolution measurement tools for characterizing the constituent properties of nano-infrastructural materials (NIMs).

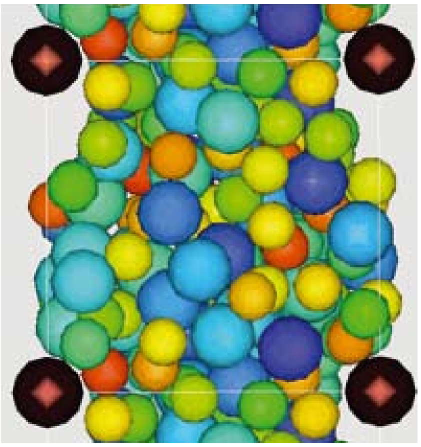
Why BFRL?

The Building and Fire Research Laboratory (BFRL) is the primary federal laboratory serving the building and fire safety industries. This strategic goal leverages the BFRL core competency in performance, durability, and service life prediction of building materials. BFRL's research in sustainability decision analysis tools and in high performance construction and building materials has been ongoing for several decades, and is internationally recognized. Industrial customers continue to recognize BFRL's world class expertise in advancing the measurement science of infrastructure materials. This recognition is evidenced by their willingness over the last two decades to establish and support ongoing NIST/industry consortia, which have as their objectives creating and validating the measurement science necessary to effect reliable sustainability decisions for infrastructure materials.

CONTACT: DR. JONATHAN MARTIN
jonathan.martin@nist.gov

Service Life Prediction of Concrete Building and Infrastructure Materials

This program will develop and implement the enabling measurement science that will give the concrete industry and state and federal government agencies the predictive capability upon which they can base the use of performance-based standards and specifications in key technical areas.



A computer model for predicting the flow properties of high performance concrete (HPC) aimed at designing HPC mixtures with optimum performance, both in the fresh and hardened states.

The overarching problem for the U.S. cement and concrete industry is that either relevant performance-based standards do not exist or that the performance-based standards that do exist are not built upon measurements that reliably predict real performance. This problem becomes evident in the technical problems plaguing the cement and concrete industry and concrete construction users and owners. The main problem is concrete durability, which needs predictive tests for the many new materials being produced, and assured longer service life. Some of these new materials include nanoadditives, whether to the liquid part of concrete (water-filled pore space), or the solid part (a complex composite of cement, hydration products, sand, and gravel), or the interface between the two, which is very large in concrete and crucially affects properties like shrinkage and ionic transport.

But concrete durability is just a part of the larger problem of concrete sustainability—trying to make and use concrete that has less of an environmental impact, uses less energy and produces less carbon dioxide, yet at the same time continues to meet or exceed expectations as the main construction material used in a rapidly-growing world. A large part of sustainability efforts in the cement and concrete industry is focused on increasing the use of fly ash and other waste-stream materials as substitutes for cement. This will reduce the need for cement and safely recycle coal combustion products, yet at the same time will improve the properties of concrete, including durability, to rebuild the nation's physical infrastructure with more sustainable materials.

Building performance prediction capabilities for cement-based materials is a challenging task due to the complexity of these materials. It is known that the materials industry in general needs performance prediction capability, which for complex modern materials (among which concrete is arguably the most complex) can only be supplied by computational materials science/engineering models or what is called an Integrated Computational Materials Engineering (ICME).[1] Therefore, the technical idea that underlies this research program is to use a combination of experimental and computational materials science/engineering, in an ICME approach, to develop performance prediction capability for selected major problems encountered by the U.S. concrete industry and in major national problems involving sustainable transportation infrastructure rebuilding and sustainable nuclear waste containment structures and new nuclear facilities.

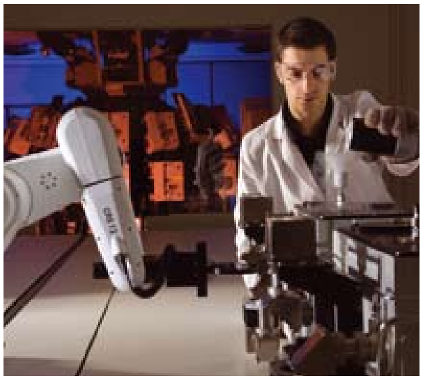
The impact of success in improving the sustainability of concrete will include: satisfying the construction needs of a growing U.S. and world economy while minimizing increase in CO_2 emissions; close to 100% recycling of fly ash, minimizing land-fill disposal; improving the performance and durability of concrete used in the infrastructure; and minimizing the CO_2/ton of cementitious material used in concrete.

CONTACT: DR. EDWARD GARBOCZI
edward.garboczi@nist.gov

Service Life Prediction of High Performance Polymers and Composites

Polymeric materials are used in the construction and building industries in a myriad of applications including protective coatings, siding, roofing, windows, doors, pipes, and geotextiles. They can be combined with fibers to form composites that have enhanced properties, enabling them to be used as structural and load-bearing members. Polymers offer many advantages over conventional materials including lightness, corrosion resistance, and ease of processing and installation.

There is currently no established, scientifically-based methodology for accurately and quantitatively predicting life cycle performance of polymeric construction materials in their end-use environment. The addition of nanoparticles to polymeric matrices further increases the difficulty of predicting life cycle performance. Degradation and nanoparticle release phenomena in nanostructured materials are inherently complex and involve numerous component interactions and multifunctional (chemical, physical, and mechanical) responses that operate over extremely large length and time scales. Nanoscale materials also possess unique properties (high surface area, high surface reactivity, and large interparticle forces) that affect many initial and long-term properties. Thus, new metrologies and methodologies that are radically different from the approaches currently used are required to obtain the necessary data for accurately modeling lifetimes and particle release behavior in new nanostructured materials.



The goal of BFRL's Automated Analytical Laboratory (AAL) is to automate and accelerate analytical measurements on polymeric specimens following exposure to various exposure environments.

[1] ICME, Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security, National Research Council, *National Academies Press*, 2008

In 2006, BFRL became the first research team to successfully and quantitatively link field and laboratory exposure results for an unfilled, model epoxy coating using a reliability-based methodology. Success in applying this methodology in predicting the service life of the epoxy coating has provided BFRL with an opportunity to move into the study of nanostructured systems, which includes polymers filled with nanoscale materials. Measurement science is being developed by BFRL researchers over a wide range of length and time scales to enable quantitative prediction of the life cycle performance[1] of nanostructured polymeric materials.

The linkage between field and laboratory exposures is studied using a reliability-based methodology for the three major classes of polymers: thermoset, thermoplastic, and elastomers. High resolution microscopy, spectroscopy and nanomechanical testing devices are being used to elucidate the effects that nanofillers have on the chemical and physical properties of nanomaterials, and as well as on the service lives of filled polymer systems. Temperature, relative humidity, and spectral UV are the primary environmental factors of interest. BFRL is focusing on metal oxide particles and carbon nanotubes, which are nano-scale fillers of interest in many structural applications.

Release of nanoparticles occurs in-service via environmental degradation and incineration through thermal, chemical, mechanical, and photolytic decomposition of nanostructured polymeric materials. The release rates and properties of these nanoparticles could have environmental, health and safety impacts. BFRL is quantitatively measuring release rates, chemical compositions, morphologies, and size distributions of aerosolized nanoparticles, using a number of advanced methods. Total mass loss and depletion of nanostructured materials during environmental exposure is being characterized with high resolution nano-gravimetry and infrared spectroscopy. Such models will be instrumental in designing improved nanocomposite materials.

[1] Life cycle is defined as material performance from manufacturing to decommissioning/disposal.

CONTACT: DR. JOANNIE CHIN
joannie.chin@nist.gov

Reduced Flammability of Materials

The phenomena associated with fire are inherently stochastic, complex and dynamic. To successfully address these challenges, BFRL is providing industry with measurement tools capable of accurately predicting the flammability behavior of materials over a multiplicity of time and length scales. Furthermore, developing the measurement science tools to enable industry to accurately evaluate the sustainability of fire safe products, especially those based on nano-materials, is primarily impeded by the lack of data available on their sustainability, i.e., their environmental, health and safety performance,

BFRL works with the U.S. mattress industry to develop the technical underpinnings for a mattress/ foundation standard that would serve as the basis for limiting the consequences of residential bed fires.

manufacturability, aging and recyclability. The challenge of coupling the difficult fire problem to the equally complex sustainability analysis is considerable.

This program is focused on three specific thrusts: 1) development of validated bench scale flammability measurement methods, 2) evaluation of new methods and materials for fire safe products and 3) a critical assessment of the sustainability of new fire safe approaches. The program will provide a competitive advantage in international markets where the new bench scale measurement methods and sustainable flame retardant approaches will enable U.S. companies to develop sustainable, cost effective, fire safe products.

Recent results of this program have led to two important impacts: 1) the promulgation of a National Mattress Flammability Standard, and 2) the development, by the polymer industry, of the first new non-halogen flame retardant system in decades based on nanoadditives.

CONTACT: DR. JEFFREY GILMAN
jeffrey.gilman@nist .gov